SYMBOL MANIPULATION AND APPLIED MATHEMATICS

FINAL REPORT

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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

An algorithm was developed to symbolically compute the infinitesimal Lie symmetries of a system of partial differential equations. A theory based on simple geometric intuition was developed for using variational problems to generate numerical grids. Symbolic algorithms were developed for transforming the variational problems to FORTRAN subroutines.

A theory is being developed for differencing general elliptic problems in general coordinates (needed when general numerical ~~grids~~ are used). Symbolic algorithms are also being developed for differencing such problems.

All symbolic algorithms have been implemented in MACSYMA and some are being submitted to the MACSYMA share library. The FORTRAN code that was generated is being used in production modeling codes.

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THE REPORT

The research which was supported by this grant had two main objectives, including the development of symbol-manipulation algorithms and the application of those algorithms to applied problems. Two main areas were studied: 1) the calculation of symmetries for systems of differential equations; and 2) the generation of FORTRAN code. The FORTRAN code was for use in numerical grid generation and for solving hosted equations on the generated grids. (Note: the work described here was carried out with partial support from the University of New Mexico, Army Research Office (this contract), and Ecodynamics Research Associates.)

A heuristic (algorithm for the polynomial case) was developed to compute the symmetries for a system of partial differential equations (PDE's). The heuristic was implemented as a small library of MACSYMA functions. The programs are run by creating a small file that contains lists of the dependent and independent variables and a list of the partial (or ordinary) differential equations. Also, there are a few parameters that must be set to control the solver. All of these instructions are in top-level MACSYMA notation, and thus user friendly. For simple PDE's, the program completely solves for the infinitesimal Lie point symmetries, which form a Lie algebra. Output form the program is a basis of the Lie algebra in standard first-order PDE notation. If the program cannot solve the problem completely, it summarizes its partial results, presents those results to the user and saves them in a file. There are utilities for reloading the results into MACSYMA, interactively solving part of the problem, and then restarting the automatic solver. This can be repeated as often as it is needed.

At the time these programs were completed, the MACSYMA group at Symbolics showed no interest in installing them in MACSYMA. In the summer of 1989, I attended (by invitation) the Workshop on Symbolic Computation Methods in Partial Differential Equations, held at the Institute for Mathematics and its Applications. Several programs for computing symmetries were discussed at this conference. It became apparent that my algorithms are competitive with, and in some ways better than, those presented by other codes. In addition, I believe my codes are significantly more user friendly than the others that were presented. Consequently, I contacted the MACSYMA group at Symbolics and we have agreed to install my programs in the MACSYMA library. During the workshop, I made several informal arrangements to work with others (F. Schwarz and W. Hereman) on extending symmetry algorithms. I encourage students to work in this area.

A masters student (in physics) extended my programs to calculate general (Lie-Backlund) symmetries and used the resulting code to compute symmetries for some examples for a professor in the Physics Department. This was his first programming experience, and consequently the programs are not sufficiently user friendly to distribute.

A related project, which implemented a Lie series package for doing perturbation and normal form calculations in MACSYMA, was carried out without support from this contract.

The numerical grids project is complete. The grid-generation algorithms that were studied are called "variational." These algorithms are based on minimizing integrals that control the length of grid lines (sometimes called smoothness), areas or volumes of grid cells, and the angles between grid lines. The integrands for the variational problems are created by

using simple geometric intuition. The symbol-manipulation algorithms start with the integrand for a variational problem, create the Euler-Lagrange equations (which are typically highly nonlinear), discretize those equations by using central differences, and then create the formulas for evaluating the stencils (coefficients) of the difference equations. The inputs for the symbol-manipulation programs are an integrand for a variational problem in high-level MACSYMA notation, the physical and logical coordinates, a notation for the indices to be used in the FORTRAN code, and a few parameters. The output of the symbol-manipulation programs is a complete FORTRAN subroutine. The symbol-manipulation programs take care of declaring the variables and arrays, creating loops, etc. The subroutines will compile under the UNIX f77 -u command, where all variables must be declared. The final step is to install the subroutines in a full grid-generation program. The subroutines have been generated and incorporated into several programs that are used at Ecodynamics, including some programs that are now sold commercially.

Although the symbol-manipulation programs are user friendly and complete, they are restricted to variational grid-generation problems, therefore, not all of the programs are appropriate for the MACSYMA library. However, the utilities which are appropriate will be installed in the library over the next year or two.

The progress made in this project is illustrated by the following example. First a FORTRAN subroutine for the Thompson smoothness algorithm in three dimensions was generated. MACSYMA took about 60 cpu hours to create this subroutine, because the subroutine was over 1800 lines long, it took over one cpu hour to compile. On the other hand, the symbol-manipulation code was written in about two weeks. The subroutine was used in a production code where it proved to be effective in generating grids. Consequently, further work was done to improve both the symbol manipulation algorithm and the generated FORTRAN code. After about a year, we were able to generate an equivalent subroutine in a few cpu minutes. The subroutine was about 180 lines long and, of course, it used in a small fraction of the time used by the large subroutine. The answers that were produced by the two subroutines were, essentially, identical.

The generation of FORTRAN code needed for solving hosted equations (typically PDE's describing fluid flow, electric fields, etc.) was started near the end of the contract. Shortly after the contract ended, we generated FORTRAN code for solving general second-order elliptic PDE's with general Robin boundary conditions. Most of the symbol code is good for any dimension, and complete FORTRAN code can be written for dimensions one, two, and three. The three-dimensional FORTRAN code is over 20 printed pages long. This does not include code for computing metrics when the numerical grids have a special structure.

The generated code is used for calculating the coefficients of a finite-difference approximation of PDE's and boundary conditions. The strategy that was used for the finite differences was based on a "staggered" grid with a finite-volume approach. Thus, in three dimensions, there are four interlaced grids, including one for volume centered quantities such as the solution values, and three for cell-face centered quantities such as fluxes and averaged variables. The finite-difference schemes are second order, nearest neighbor, and symmetric in the interior of the region. (I have nearly completed a proof which demonstrates that the symmetry

cannot be extended to the boundary and preserve the other properties. If the boundary conditions are simplified slightly, then the symmetry can be extended.) Both linear and harmonic averaging is available for interpolating the coefficients of the PDE's. Generating the overall code logic and loop structures were major obstacles in this project.

During this contract period, I communicated with the MACSYMA (Symbolics), Maple, and Scratchpad groups on a regular basis. My input had significant impact on the implementation of a new operator definition for derivatives in MACSYMA, the algorithms in the linear equation solver in Maple, and the current development of a "functional expression" data type in Scratchpad.

This work has had significant impact on undergraduate and graduate education, and the education of my colleagues. I have given numerous expository talks (see below) and several research talks, and I have published one short expository paper. I have shared information on symbol manipulation with a large number of people (my office is always open for consultation). All of my graduate students have been required to use a symbol manipulator in their research. I have taught two, full-semester, symbol-manipulation courses at UNM. As part of my teaching preparation, I have had extensive discussions with a colleague who is writing an advanced undergraduate-level text for symbol manipulation. I believe the discussions are having a positive impact on the book.

SUPPORTED PERSONNEL

Professor Stanly Steinberg was supported on this contract. In addition, the students M. Wester, M. Florence, R. Mertig, and D. Collett were supported. M. Wester is writing his thesis, M. Florence is beginning her thesis work, R. Mertig finished his Master's Degree, and D. Collett obtained his BS Degree. In addition, students who were not supported, worked on problems directly related to this contract.

SUPPORTED STUDENTS

Mr. Michael Wester, Ph.D. in progress, Symbolic Computation of Matrix Eigenvalues and Eigenvectors. Talks: *Expression Swell Analysis of the Computation of Matrix Characteristic Polynomials*, invited talk, Special Session on Symbolic Computing, Sixth Army Conference on Applied Mathematics and Computing, University of Colorado, May, 1988.

Ms. Megan Florence, Masters Practicum, 1986, Symbolic Ordinary Differential Equation Solver and Analyzer. Publication: *MACSYMA-izing FORTRAN Code*, MACSYMA Newsletter, **III-3** (1986), 8-12. Ph.D. in progress, Icosahedral Symmetry in Physics and Chemistry Using Symbolic Techniques.

Mr. David Scott-Collett, Undergraduate Project, 1987, High School Resource Material for Maple.

Mr. Rolf Mertig, Master Project (in physics), 1987, The Computation Higher-Order Symmetries for Systems of Partial Differential Equations Using MACSYMA.

STUDENTS
(Work is related but not supported.)

Ms. Elena Solana, Masters Practicum, 1985, Symbolic Separation of Variables in Partial Differential Equations.

Dr. José Castillo, Ph.D., 1987, Numerical Grid Generation Using Variational Techniques. Publications (7): Mathematical Aspects of Numerical Grid Generation I, International Conference on Numerical Grid Generation in Computational Fluid Dynamics, Landshut, 1986. Thesis paper accepted in SIAM Journal of Statistic and Scientific Computing.

Mr. Tom Robey, Ph.D., Mixed Finite-Element Algorithms, Efficient Formulations, Use of Symbolic Techniques. Has a paper published in the International Journal for Numerical Methods in Engineering, 1988.

Dr. Pat Knupp, Ph.D. 1989, Robust Grid Generation. One paper accepted for publication in Computational Methods in Applied Mechanical Engineering, submitted another paper.

PUBLICATIONS

The following publications and reports were prepared with partial support from this grant. The numbers agree with those in my vita.

42. (With P.J. Roache) *Variational grid generation*, Numerical Methods for Partial Differential Equations, **2** (1985), 71-96.

44. (With J.E. Castillo and P.J. Roache) *Mathematical aspects of variational grid generation II*, Journal of Computational and Applied Mathematics, **20** (1987), 127-135.

45. (With P.J. Roache) *A toolkit of symbolic manipulation programs for variational grid generation*, AIAA Paper No. 86-0241, Proceedings of the AIAA 24th Aerospace Sciences Meeting, Reno, Nevada, 1986. Also, Transactions of the Fourth Army Conference on Applied Mathematics and Computation, Ithaca, NY, 1986. Also, Proceedings of the Coupling Symbolic and Numeric Computing in Knowledge Based Systems Workshop, Boeing Computer Services, Seattle, WA, 1987.

46. (With P.J. Roache) *Grid generation: a variational and symbolic-computation approach*, Proceedings of the Numerical Grid Generation in Fluid Dynamics Conference, Landshut, W. Germany, 1986.

48. (With J.E. Castillo and P.J. Roache) *On the folding of numerically generated grids: use of reference grid*, Communications in Applied Numerical Methods, **4** (1988), 471-481.

49. *Overview of symbol manipulation*, CWI Quarterly, **1** (1988), 65-72.

50. (With P.J. Roache and J.E. Castillo) *Parameter estimation in variational grid generation*, Applied Mathematics and Computation, **28** (1988), 155.

51. (With P.J. Roache) *Automatic generation of finite difference code* invited presentation, Symbolic Computation in Fluid Mechanics and Heat Transfer, (H.H. Bau, T. Herbert, M.M. Yovanovich, eds.), HTD-Vol. 105, AMD-Vol. 97, the Heat Transfer Division and the Applied Mechanics Division, ASME ASME Winter Annual Meeting, Chicago, IL, Nov. 1988.

PAPERS SUBMITTED FOR PUBLICATION

53. (With P.J. Roache) *Variational curve and surface grid generation.* Submitted to JCP.

WORK IN PROGRESS

54. (With P.J. Roache) *Symmetric operators in general coordinates.*

PRESENTATIONS

Oct. 85. *An Overview of Symbol Manipulation*, Joint Theoretical Seminar, UNM.

Oct. 85. (With J.E. Castillo and P.J. Roache) *On the Folding of Numerical Grids*, SIAM, Arizona State University, Tucson, AZ.

Jan. 86. (With P.J. Roache) *A Toolkit of Symbolic Manipulation Programs for Variational Grid Generation*, AIAA 24th Aerospace Sciences Meeting.

May 86. (With P.J. Roache) *A Toolkit of Symbolic Manipulation Programs for Variational Grid Generation*, Fourth Army Conference on Applied Mathematics and Computing.

June 86. (With J.E. Castillo and P.J. Roache) *On the Folding of Numerically Generated Grids: Use of Reference Grids*, 10th U.S. National Congress of Applied Mechanics, Austin, TX.

June 86. (With P.J. Roache) *Policy Recommendations for NSF Program in Computational Engineering*, NSF Workshop of Computational Engineering, University of California, San Diego, CA.

June 86. (With P.J. Roache) *Symbolic Manipulation and Computational Fluid Dynamics*, invited presentation, NSF Workshop on Computational Engineering, NSF Supercomputer Center, San Diego, CA.

July 86. (With J.E. Castillo and P.J. Roache) *Mathematical Aspects of Variational Grid Generation II*, International Congress on Computational and Applied Mathematics, University of Leuven, Belgium.

July 86. (With P.J. Roache) *Grid Generation: A Variational and Symbolic-Computation Approach*, Numerical Grid Generation in Computational Fluid Dynamics Conference, Landshut, West Germany.

April 87. *Introduction to Computer Algebra*, Southwestern Section of the MAA, Albuquerque, New Mexico.

June 87. *Evolution Equations with Generators in a Lie Algebra*, invited paper, Symmetry Methods in Differential Equations, Utah State University, Logan, UT.

Aug. 87. *Generating Subroutine Codes with MACSYMA*, invited paper, Sixth International Conference on Mathematical Modeling, St. Louis, MO.

Oct. 87. (With P.J. Roache) *Grid Generation on Surfaces and Curves*, SIAM 35th Anniversary Meeting, Denver, CO.

Oct. 87. *Symbol Manipulation in Scientific Computing*, colloquium, Michigan Technological University, Houghton, MI.

March 88. *The Symbolic-Numeric Programming Interface*, colloquium, San Diego State University, San Diego, CA.

March 88. *Variational Grid Generation*, colloquium, San Diego State University, San Diego, CA.

May 88. *A Survey of Fortran Code Generation Using MACSYMA*, invited talk, Acoustical Society of America, Seattle, WA.

July 88. (With P.J. Roache) *Anomalies in Surface Grid Generation*, First National Fluid Dynamics Conference, Cincinnati, OH.

June 88. (With P.J. Roache, D. Dietrich and M.G. Marietta) *A Boundary Fitted Coordinate Computational Model for the North Atlantic*, invited presentation, VII International Conference on Computational Methods in Water Resources, MIT, Cambridge, MA.

July 88. (With P.J. Roache) *Grid Generation on Curves and Surfaces*, Minisymposia on Mathematical Aspect of Numerical Grid Generation (organizer), SIAM Annual Meeting, Minneapolis, MN.

Dec. 88. (With P.J. Roache) *Automatic Generation of Finite Difference Code*, invited presentation, Symposium on Symbolic Computation in Heat Transfer and Fluid Mechanics, ASME Winter Annual Meeting, Chicago, IL.

PROFESSIONAL ACTIVITIES

Mar. 85. Judged the Northwestern New Mexico Regional Science and Engineering Fair.

Feb. 86. Graded the Mathematical Competition in Modeling Contest.

July 86. Attended the ACM-SIGSAM (SYMSAC '86) Symposium on Symbolic and Algebraic Computation in Waterloo, Canada.

March 87. Judged the Annual Northwestern NM Regional Science Fair.

April 87. Co-director, Institute for Computational Research.

Sept. 87. Search Committee, VP for Computing.

Sept. 87.. Chairman of the Search Committee for chairman of Computer Science Department.

March 88. Judged the Annual Northwestern NM Regional Science Fair.

July 88. Invited to participate in the Computer Algebra Systems Workshop, Colby College, Waterville, ME.

July 88. Attended the First International Joint Conference of ISSAC (Symbolic and Algebraic Computation) and AAEC (Applied Algebra, Algebraic Algorithms and Error Correcting Code), Rome.

July 88. (With José Castillo) Organized a Minisymposia at the SIAM Annual Meeting. Minneapolis, MN.

88-89. Sabbatical leave.

Sept. 88. Visit R. Jenks at IBM-Watson (by invitation). Worked on Scratchpad II.

Sept. 88. (With P.J. Roache) Anomalies in Grid Generation, Scientific Computing and Numerical Analysis Seminar, UNM.

Nov. 88. Symbolic Manipulators: MACSYMA, Maple, Reduce, SMP, MuMath, Mathematica. CHE/NE Lecture, UNM.

Dec. 88. Received a long-term loan of an IBM-RT Workstation and Scratchpad II code for symbol-manipulation research.

Mar. 89. Lie Methods in Optics. Organized a visit of Dr. K.B. Wolf of IMAS-UNAM in Mexico to the M&S and Chemistry Departments and CNLS at LANL.

Mar. 89. SIAM Conference on Domain Decomposition Methods. Attended with Pat Knupp, Tom Robey, and Pat Roache.

June 89. Workshop on Symbolic Computation Methods in Differential Equations at the IMA. Attending by invitation.

June 89. 1989 Computers and Mathematics Conference. Reviewed numerous proposals for tutorial minicourses.

June 89. Attended (by invitation only) the Workshop on Symbolic Computation Methods in Partial Differential Equations held at the Institute for Mathematics and its Applications, Minneapolis, MN.

July 89. International Symposium on Symbolic and Algebraic Computation. Will attend. **(Advised Program Committee on speakers.)**

April 90. Will organize a special session at the local AMS-SIAM meeting.

April 90. School on Group Theoretic Methods in Optics (Italy). I will give three or four lectures on Lie series.

Jan. 91. Assisting Professor Castillo in the organization of an applied mathematics meeting in Venezuela.